

Supporting Information

New Mn^{II}-Azido Coordination Polymers Based on Nicotinic/Isonicotinic Acids as Co-Ligands: Synthesis, Structure and Magnetic Properties

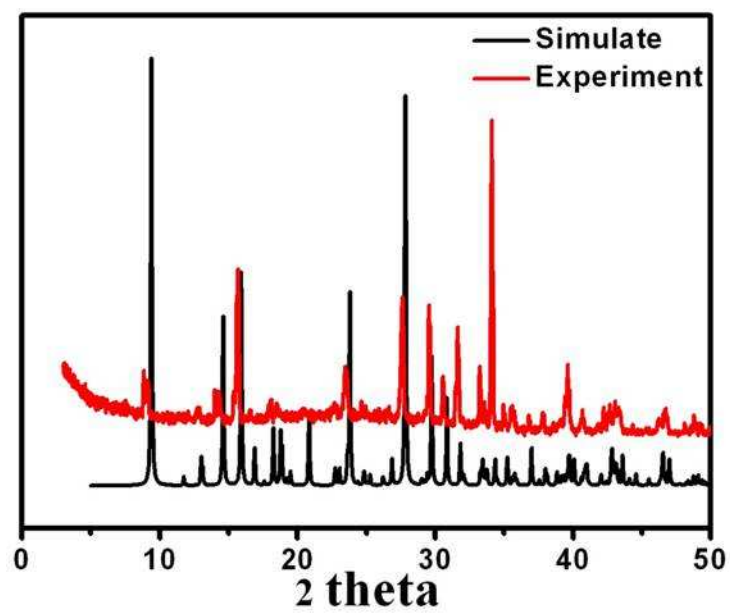
Qian Yang, Jiong-Peng Zhao, Bo-Wen Hu, Xiao-Feng Zhang and Xian-He Bu*

Department of Chemistry, Nankai University, Tianjin 300071, P. R. China

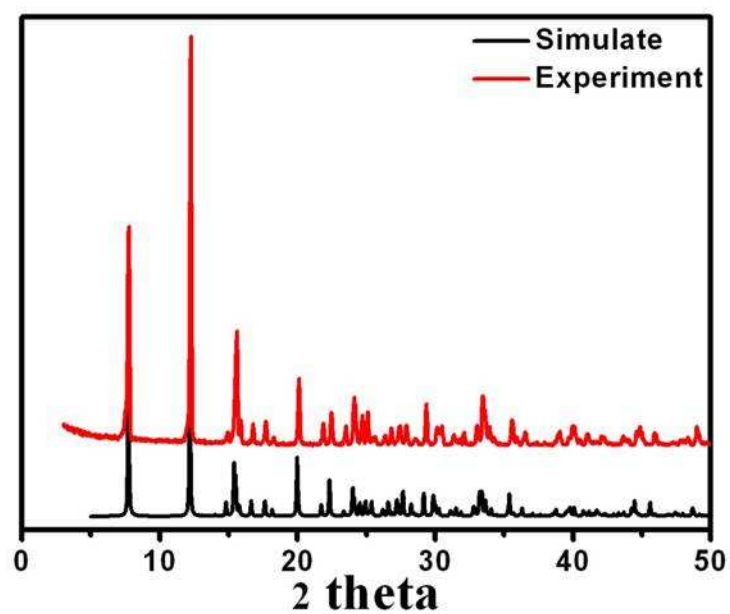
Table S1. Selected Bond Lengths [Å] and Angles [deg] for Complexes 1–2.

1			
Mn(1)-O(2)#4	2.092(2)	Mn(2)-O(1)#3	2.098(2)
Mn(1)-O(2)#5	2.092(2)	Mn(2)-N(1)	2.324(3)
Mn(1)-N(3)#6	2.278(3)	Mn(2)-N(4)	2.234(3)
Mn(1)-N(3)#7	2.278(3)	Mn(2)-N(7)	2.255(3)
Mn(1)-N(6)#8	2.288(3)	Mn(2)-N(3)#2	2.278(3)
Mn(1)-N(6)	2.288(3)	Mn(2)-N(4)#7	2.320(3)
O(2)#4-Mn(1)-O(2)#5	180.0	O(1)#3-Mn(2)-N(4)	96.62(10)
O(2)#4-Mn(1)-N(3)#6	93.47(9)	O(1)#3-Mn(2)-N(7)	90.37(9)
O(2)#5-Mn(1)-N(3)#6	86.53(9)	N(4)-Mn(2)-N(7)	96.16(10)
O(2)#4-Mn(1)-N(3)#7	86.53(9)	O(1)#3-Mn(2)-N(3)#2	92.47(9)
O(2)#5-Mn(1)-N(3)#7	93.47(9)	N(4)-Mn(2)-N(3)#2	92.89(10)
N(3)#6-Mn(1)-N(3)#7	180.0	N(7)-Mn(2)-N(3)#2	170.14(9)
O(2)#4-Mn(1)-N(6)#8	91.77(11)	O(1)#3-Mn(2)-N(4)#7	173.36(10)
O(2)#5-Mn(1)-N(6)#8	88.23(11)	N(4)-Mn(2)-N(4)#7	76.88(10)
N(3)#6-Mn(1)-N(6)#8	86.42(10)	N(7)-Mn(2)-N(4)#7	91.64(9)
N(3)#7-Mn(1)-N(6)#8	93.58(10)	N(3)#2-Mn(2)-N(4)#7	86.61(9)
O(2)#4-Mn(1)-N(6)	88.23(11)	O(1)#3-Mn(2)-N(1)	97.47(10)
O(2)#5-Mn(1)-N(6)	91.77(11)	N(4)-Mn(2)-N(1)	165.83(10)
N(3)#6-Mn(1)-N(6)	93.58(10)	N(7)-Mn(2)-N(1)	85.31(10)
N(3)#7-Mn(1)-N(6)	86.42(10)	N(3)#2-Mn(2)-N(1)	84.96(10)
N(6)#8-Mn(1)-N(6)	180.000(1)	N(4)#7-Mn(2)-N(1)	89.00(10)
#1 x-1,y+1,z	#2 -x,-y+1,-z+1	#3 -x+1,-y+1,-z+2	#4 x,y-1,z-1
#5 -x+2,-y+1,-z+2	#6 x+1,y-1,z	#7 -x+1,-y+1,-z+1	#8 -x+2,-y,-z+1
#9 x,y+1,z+1			
2			
Mn(1)-O(1)#5	2.231(2)	Mn(2)-O(2)#6	2.154(2)
Mn(1)-O(1)#6	2.232(2)	Mn(2)-O(2)#7	2.154(2)
Mn(1)-N(5)	2.145(3)	Mn(2)-N(4)#8	2.254(2)
Mn(1)-N(10)#4	2.213(3)	Mn(2)-N(4)#1	2.254(2)

Mn(1)-N(8)	2.263(2)	Mn(2)-N(8)	2.320(3)
Mn(1)-N(4)	2.267(3)	Mn(2)-N(8)#9	2.320(3)
Mn(3)-N(7)#10	2.221(3)	Mn(3)-N(2)	2.260(3)
Mn(3)-N(7)#11	2.221(3)	Mn(3)-N(1)	2.264(3)
Mn(3)-N(2)#12	2.260(3)	Mn(3)-N(1)#12	2.264(3)
N(5)-Mn(1)-N(10)#4	102.36(12)	O(2)#6-Mn(2)-O(2)#7	180.0
N(5)-Mn(1)-O(1)#5	167.60(10)	O(2)#6-Mn(2)-N(4)#8	94.18(9)
N(10)#4-Mn(1)-O(1)#5	88.87(10)	O(2)#7-Mn(2)-N(4)#8	85.82(9)
N(5)-Mn(1)-O(1)#6	92.28(10)	O(2)#6-Mn(2)-N(4)#1	85.82(9)
N(10)#4-Mn(1)-O(1)#6	165.35(10)	O(2)#7-Mn(2)-N(4)#1	94.18(9)
O(1)#5-Mn(1)-O(1)#6	76.50(8)	N(4)#8-Mn(2)-N(4)#1	180.0
N(5)-Mn(1)-N(8)	96.30(11)	O(2)#6-Mn(2)-N(8)	93.24(9)
N(10)#4-Mn(1)-N(8)	89.86(10)	O(2)#7-Mn(2)-N(8)	86.76(9)
O(1)#5-Mn(1)-N(8)	88.88(9)	N(4)#8-Mn(2)-N(8)	91.52(9)
O(1)#6-Mn(1)-N(8)	89.13(8)	N(4)#1-Mn(2)-N(8)	88.48(9)
N(5)-Mn(1)-N(4)	87.94(10)	O(2)#6-Mn(2)-N(8)#9	86.76(9)
N(10)#4-Mn(1)-N(4)	93.13(10)	O(2)#7-Mn(2)-N(8)#9	93.24(9)
O(1)#5-Mn(1)-N(4)	86.19(8)	N(4)#8-Mn(2)-N(8)#9	88.48(9)
O(1)#6-Mn(1)-N(4)	86.73(8)	N(4)#1-Mn(2)-N(8)#9	91.52(9)
N(8)-Mn(1)-N(4)	174.19(9)	N(8)-Mn(2)-N(8)#9	180.000(1)
N(7)#10-Mn(3)-N(7)#11	180.0	N(7)#11-Mn(3)-N(1)	89.11(10)
N(7)#10-Mn(3)-N(2)#12	89.86(11)	N(2)#12-Mn(3)-N(1)	91.70(10)
N(7)#11-Mn(3)-N(2)#12	90.14(11)	N(2)-Mn(3)-N(1)	88.30(10)
N(7)#10-Mn(3)-N(2)	90.14(11)	N(7)#10-Mn(3)-N(1)#12	89.11(10)
N(7)#11-Mn(3)-N(2)	89.86(11)	N(7)#11-Mn(3)-N(1)#12	90.89(10)
N(2)#12-Mn(3)-N(2)	180.000(1)	N(2)#12-Mn(3)-N(1)#12	88.30(10)
N(7)#10-Mn(3)-N(1)	90.89(10)	N(2)-Mn(3)-N(1)#12	91.70(10)
N(1)-Mn(3)-N(1)#12	180.0		
#1 x,y+1,z	#2 -x+2,y-1/2,-z+3/2	#3 x+1,-y+3/2,z+1/2	#4 -x+1,y-1/2,-z+1/2
#5 x-1,-y+3/2,z-1/2	#6 -x+2,y+1/2,-z+3/2	#7 x-1,-y+5/2,z-1/2	#8 -x+1,-y+2,-z+1
#9 -x+1,-y+3,-z+1	#10 x,y-1,z	#11 -x+2,-y+2,-z+1	#12 -x+2,-y+1,-z+1
#13 -x+1,y+1/2,-z+1/2			



(a)



(b)

Figure S1. The XRPD diagrams for (a) complex 1; (b) complex 2.

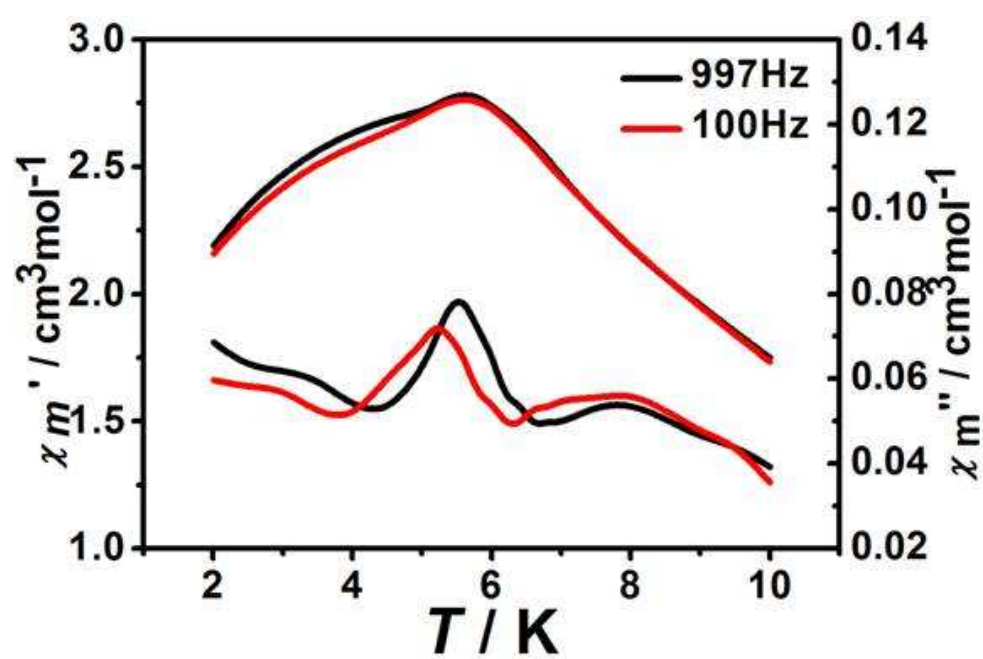


Figure S2. The *ac* magnetic susceptibility curves at different frequencies for complex **1**.

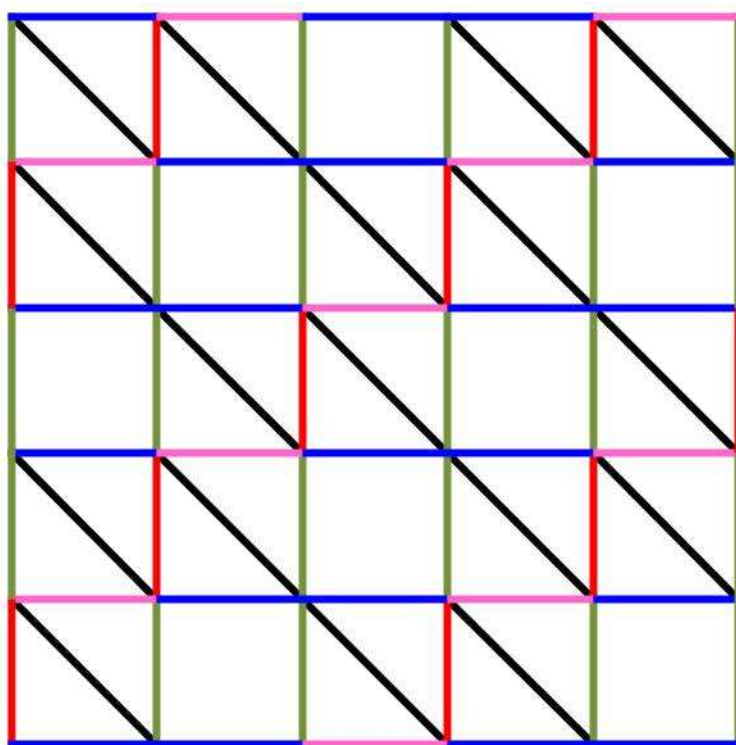


Figure S3. The magnetic network of complex **1**. (The lines in different color are the different magnetic transmit constructed by the azido between Mn^{II} ions.)

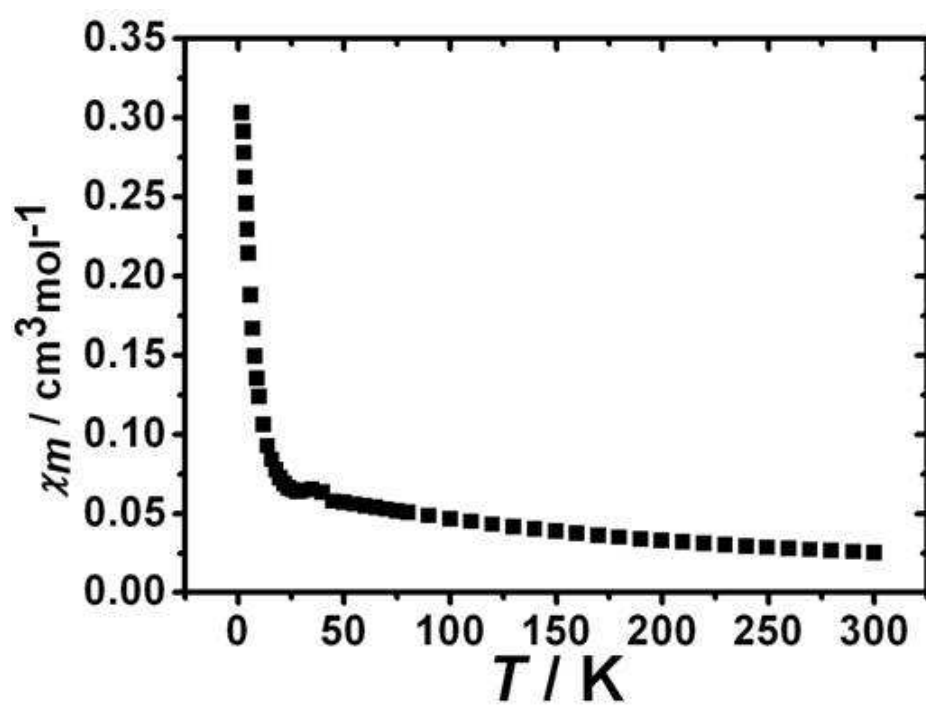


Figure S4. The χ_m vs. T plots of **2** at 2 kOe.

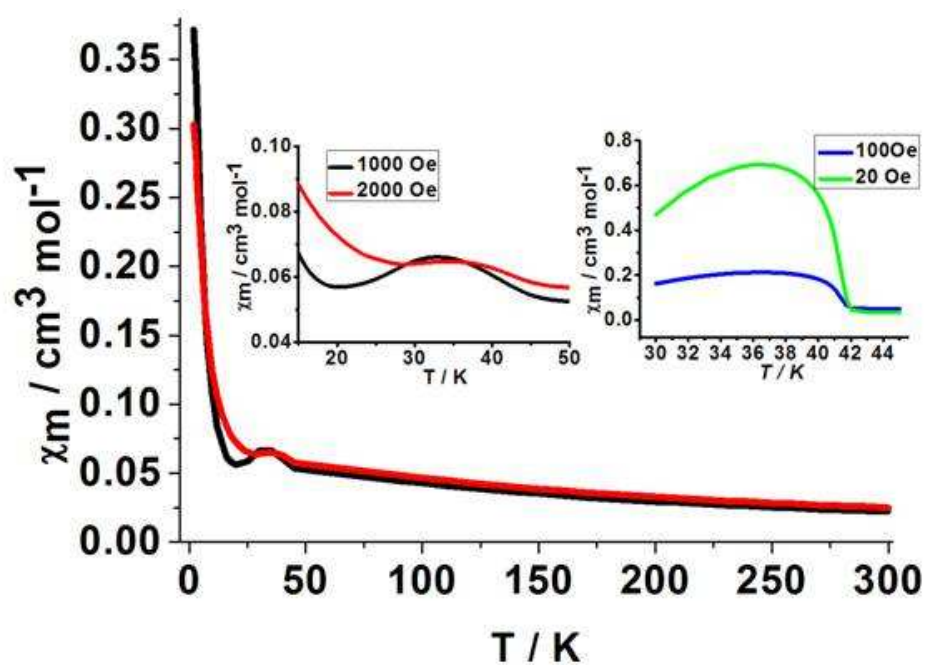


Figure S5. The χ_m vs. T curves of **2** at 1 kOe and 2 kOe. Inset: curves of χ_m vs. T under various fields.